Excerpt from the Proceedings of the COMSOL Conference 2024 Florence

REFERENCES

MEMS Gas-Chromatograph Pre-Concentrator Multiphysics Simulation

G. Spinola Durante, A. Hoogerwerf, D. Bayat Zaman

Swiss Center for Electronics and Microtechnology (CSEM), Neuchâtel,

Thermal and flow models required experimental validation of material properties of Tenax® porous material pellets. A flow model has been implemented with calibrated parameters based on the heating setup of a cube filled with Tenax®. Gas-flow behavior of Tenax® porous material has been estimated based on literature flow data for a round pipe filled with Tenax® particles and accordingly simulated and calibrated with a model [2, 3]. Selected physics have been included in the chip model: heat transfer in solid and fluids, laminar flow, with porous flow in Tenax® and electrical current in shells (2D-layer) to model the pre-concentrator heater. The selected physics are also coupled together to correctly compute ohmic losses in the heater and non-isothermal flow due to strong thermal gradients in the model as shown in Fig. 1 (a, b).

1. High-performance MEMS-based gas chromatography column with integrated micro heater https://link.springer.com/article/10.1007/s00542-010-1165-y

2. Tenax® TA Adsorbent Resin Specifications

https://www.sisweb.com/index/referenc/tenaxtam.htm#4

3. COMSOL Blog: Modeling Darcian and Non-Darcian Flow in Porous Media https://www.comsol.com/blogs/modeling-darcian-and-non-darcian-flow-in-porous-media

FIGURE 1 (a, b). MEMS pre-concentrator chip temperature, (c): optimized heater current density.

MEMS Gas-Chromatograph (GC) is a key system for a miniaturized planetary (Mars) atmospheric life detector [1]. A methodology is shown to optimize the preconcentrator MEMS chip design. The chip absorbs VOCs in Tenax® layer and fast desorbs them by heating. This development was funded by ESA.

The objective of this simulation model is to enhance the thermal behavior of a MEMS Gas-Chromatograph (GC) pre-concentrator of Volatile Organic Compounds (VOCs).

Precise and rapid temperature control is essential for optimal VOC desorption from the Tenax® polymer filling the pre-concentrator chip cavity. By inducing a fast-heating pulse, we release highly time-concentrated VOCs into the carrier gas (Helium) exiting the pre-concentrator, leading to increased accuracy of VOCs detection.

The simulation plays a critical role in estimating the heater geometry, its maximum voltage and current density, thermal time constants, and spatial temperature uniformity within the Tenax® polymer material. The chip design optimization comes with a few challenges i.e. voltage is limited to 28V and current must be lower than the heater electro-migration limit. Tenax® temperature uniformity is reduced by heatsinking of the chip to its surroundings. Chip size is limited due to yield & costs issues. Tenax® target heating is 280-300°C in <5s in >70% volume.

Introduction

Methodology

The model solves in 1h40m on a Linux® Server and helps to quantify the Tenax® spatial (volume) and temporal temperature evolution in form of relative volume histogram snapshots for specific time-slices. The initial symmetric heater and thermal connection design was delivering 30% of Tenax® temperature uniformity in 20°C range, around the peak. It gave insight how to effectively optimize the asymmetric heater design, its position on chip and resulted in Tenax® heating speed-up reaching a range of 265-285°C in \sim 2.5s within >64% of the volume (Fig. 2a). The heater is operated at a power of ~27W. A different Tenax® configuration, based on same chip size and heater improved the Tenax[®] heating range of 275-295°C in \sim 3.1s within >84% of the volume (Fig. 2b). Finally, the heater is operating with a current density of ~3E5A/cm2 and well below the limit (Fig. 1c).

Results

FIGURE 2 (a). Tenax® temperature distribution optimized, (b): Tenax® temperature distribution improved uniformity.

